

=> d hist

(FILE 'HOME' ENTERED AT 10:12:53 ON 10 FEB 2004)

FILE 'STNGUIDE' ENTERED AT 10:13:05 ON 10 FEB 2004

FILE 'REGISTRY' ENTERED AT 10:14:49 ON 10 FEB 2004

E ASMN2/MF  
L1 1 S E3  
E MN2P/MF  
L2 1 S E3

FILE 'CAPLUS' ENTERED AT 10:16:23 ON 10 FEB 2004

L3 43 S L1  
L4 1 S L3 AND (LITHIUM OR LI)  
L5 48 S L2  
L6 0 S L5 AND (LITHIUM OR LI)  
L7 0 S L5 AND ELECTRODE#  
L8 0 S L5 AND INTERCALAT####  
L9 0 S L1 AND ELECTRODE#  
L10 0 S L1 AND INTERCALAT####  
S 12005-88-8/REG#

FILE 'REGISTRY' ENTERED AT 10:30:27 ON 10 FEB 2004

L11 1 S 12005-88-8/RN

FILE 'CAPLUS' ENTERED AT 10:30:27 ON 10 FEB 2004

L12 88 S L11  
L13 0 S L12 AND (ELECTRODE# OR ANODE#)  
S 12006-15-4/REG#

FILE 'REGISTRY' ENTERED AT 10:31:59 ON 10 FEB 2004

L14 1 S 12006-15-4/RN

FILE 'CAPLUS' ENTERED AT 10:31:59 ON 10 FEB 2004

L15 456 S L14  
L16 5 S L15 AND (ELECTRODE# OR ANODE#)  
S 12006-40-5/REG#

FILE 'REGISTRY' ENTERED AT 10:34:58 ON 10 FEB 2004

L17 1 S 12006-40-5/RN

FILE 'CAPLUS' ENTERED AT 10:34:58 ON 10 FEB 2004

L18 267 S L17  
L19 0 S L18 AND (ELECTRODE# OR ANODE#)  
L20 7 S L18 AND (LITHIUM OR LI)  
S 12014-28-7/REG#

FILE 'REGISTRY' ENTERED AT 10:40:20 ON 10 FEB 2004

L21 1 S 12014-28-7/RN

FILE 'CAPLUS' ENTERED AT 10:40:21 ON 10 FEB 2004

L22 210 S L21  
L23 0 S L22 AND (ELECTRODE# OR ANODE#)  
L24 4 S L22 AND (LITHIUM OR LI)  
S 12133-44-7/REG#

FILE 'REGISTRY' ENTERED AT 10:46:34 ON 10 FEB 2004

L25 1 S 12133-44-7/RN

FILE 'CAPLUS' ENTERED AT 10:46:35 ON 10 FEB 2004

L26 283 S L25  
L27 2 S L26 AND (ANODE# OR ELECTRODE#)  
S 12254-85-2/REG#

FILE 'REGISTRY' ENTERED AT 10:48:07 ON 10 FEB 2004

L28 1 S 12254-85-2/RN

FILE 'CAPLUS' ENTERED AT 10:48:07 ON 10 FEB 2004

L29 32 S L28  
L30 0 S L29 AND (ELECTRODE# OR ANODE#)  
L31 0 S L29 AND BATTER###  
S 12263-33-1/REG#

FILE 'REGISTRY' ENTERED AT 10:49:28 ON 10 FEB 2004

L32 1 S 12263-33-1/RN

FILE 'CAPLUS' ENTERED AT 10:49:29 ON 10 FEB 2004

L33 31 S L32  
L34 0 S L33 AND (ELECTRODE# OR ANODE# OR BATTER###)

> d hist

(FILE 'HOME' ENTERED AT 12:14:25 ON 11 FEB 2004)

FILE 'STNGUIDE' ENTERED AT 12:14:32 ON 11 FEB 2004

FILE 'REGISTRY' ENTERED AT 12:14:43 ON 11 FEB 2004

E COP3/MF

L1 1 S E3

FILE 'REGISTRY' ENTERED AT 12:16:23 ON 11 FEB 2004

L2 STR 12187-17-6

L3 0 S L2 EXA SAM

FILE 'CAPLUS' ENTERED AT 12:16:46 ON 11 FEB 2004

L4 20 S L1 AND STRUCTURE

L5 13 S L4 AND CRYSTAL####

L6 0 S L5 AND CU2S

L7 9 S L1 (P) STRUCTURE

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YOU HAVE REQUESTED DATA FROM 9 ANSWERS - CONTINUE? Y/(N):y

L7 ANSWER 1 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2000:342861 CAPLUS

DOCUMENT NUMBER: 133:67806

TITLE: Crystal structure and properties of some filled and unfilled skutterudites: GdFe<sub>4</sub>P<sub>12</sub>, SmFe<sub>4</sub>P<sub>12</sub>, NdFe<sub>4</sub>As<sub>12</sub>, Eu<sub>0.54</sub>Co<sub>4</sub>Sb<sub>12</sub>, Fe<sub>0.5</sub>Ni<sub>0.5</sub>P<sub>3</sub>, CoP<sub>3</sub>, and NiP<sub>3</sub>

AUTHOR(S): Jeitschko, Wolfgang; Foecker, Aloys J.; Paschke, Dirk; Dewalsky, Martin V.; Evers, Ch. B. H.; Kunnen, Bernd; Lang, Arne; Kotzyba, Gunter; Rodewald, Ute Ch.; Moller, Manfred H.

CORPORATE SOURCE: Anorganisch-Chemisches Institut der Universitat, Munster, D-48149, Germany

SOURCE: Zeitschrift fuer Anorganische und Allgemeine Chemie (2000), 626(5), 1112-1120  
CODEN: ZAACAB; ISSN: 0044-2313

PUBLISHER: Wiley-VCH Verlag GmbH

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The new cubic compound Fe<sub>0.5</sub>Ni<sub>0.5</sub>P<sub>3</sub> ( $\alpha$  775.29(5)pm) as well as the known compds. CoP<sub>3</sub> and NiP<sub>3</sub> were synthesized from the elemental components using Sn as a flux. Their skutterudite (CoAs<sub>3</sub>) type structures were refined from single-crystal x-ray data. The new compound GdFe<sub>4</sub>P<sub>12</sub> was prepared by reaction of an alloy Gd<sub>1/3</sub>Fe<sub>2</sub>Y<sub>3</sub> with P in a Sn flux. Its cubic filled skutterudite (LaFe<sub>4</sub>P<sub>12</sub> type) structure was refined from single-crystal x-ray data:  $a$  779.49(4) pm,  $R = 0.019$  for 304 structure factors and 11 variable parameters. SmFe<sub>4</sub>P<sub>12</sub> shows Van Vleck paramagnetism while GdFe<sub>4</sub>P<sub>12</sub> is a soft ferromagnet with a Curie temperature of

Tc = 22(5) K. Both are metallic conductors. The new isotypic polyarsenide NdFe<sub>4</sub>As<sub>12</sub> (a 830.9(1) pm) was obtained by reacting NdAs<sub>2</sub> with Fe and As in the presence of a NaCl/KCl flux. The new isotypic polyantimonide Eu<sub>0.54</sub>(1)Co<sub>4</sub>Sb<sub>12</sub> (a 909.41(8) pm) was prepared by reaction of EuSb<sub>2</sub> with Co and Sb. Its structure was refined from single-crystal x-ray data to a residual of 0.024 (137 F values, 12 variables). A comparison of the Fe-P and P-P bond lengths in the compds. AFe<sub>4</sub>P<sub>12</sub>, where the A atoms (A = Ce, Eu, Gd, Th) have differing valencies, suggests that the Fermi level cuts through Fe-P bonding and P-P antibonding bands.

- IT Crystal structure  
(of Group VIII pnictides)
- IT Curie temperature (paramagnetic)  
Electric resistance  
Paramagnetism  
(of iron gadolinium/samarium phosphides)
- IT 65035-81-6P, Iron samarium phosphide (Fe<sub>4</sub>SmP<sub>12</sub>) 276693-77-7P, Gadolinium iron phosphide (GdFe<sub>4</sub>P<sub>12</sub>)  
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation and crystal structure and elec. conductivity)
- IT 12187-17-6P, Cobalt phosphide (CoP<sub>3</sub>) 12192-07-3P, Nickel phosphide (NiP<sub>3</sub>) 276693-78-8P, Iron neodymium arsenide (Fe<sub>4</sub>NdAs<sub>12</sub>) 276693-79-9P 276693-80-2P, Iron nickel phosphide (Fe<sub>0.5</sub>Ni<sub>0.5</sub>P<sub>3</sub>)  
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation and crystal structure of)
- IT 7439-89-6, Iron, reactions 7440-00-8, Neodymium, reactions 7440-02-0, Nickel, reactions 7440-19-9, Samarium, reactions 7440-31-5, Tin, reactions 7440-36-0, Antimony, reactions 7440-38-2, Arsenic, reactions 7440-48-4, Cobalt, reactions 7723-14-0, Phosphorus, reactions 12512-02-6, Neodymium arsenide (NdAs<sub>2</sub>) 12739-23-0, Iron 67 nickel 33 (atomic) 59984-51-9, Gadolinium 33 iron 67 (atomic) 69459-69-4 276693-81-3  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reactant for preparation of cobalt/iron/nickel pnictides with/without other metals)

REFERENCE COUNT: 65 THERE ARE 65 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1999:254366 CAPLUS

DOCUMENT NUMBER: 130:359907

TITLE: Electronic structure and thermoelectric prospects of phosphide skutterudites

AUTHOR(S): Fornari, Marco; Singh, David J.

CORPORATE SOURCE: C.S.I. George Mason University, Fairfax, VA, 22030-4444, USA

SOURCE: Physical Review B: Condensed Matter and Materials Physics (1999), 59(15), 9722-9724  
CODEN: PRBMD0; ISSN: 0163-1829

PUBLISHER: American Physical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The prospects for high thermoelec. performance in phosphide skutterudites are studied based on 1st-principles calcns. We find that stoichiometric CoP3 differs from the corresponding arsenide and antimonide in that it is metallic. As such, the band structure must be modified if high thermopowers are to be achieved. In analogy to the antimonides, it is expected that this may be done by filling with La. Calcns. for LaFe4P12 show that a gap can in fact be opened by La filling, but that the valence band is too light to yield reasonable p-type thermopowers at appropriate carrier densities; n-type La-filled material may be more favorable.

IT Thermoelectric materials  
(electronic structure and thermoelec. prospects of phosphide skutterudites)

IT Band structure  
Density of states  
Electronic structure  
(of thermoelec. phosphide skutterudites)

IT 12187-17-6, Cobalt phosphide (CoP3) 65035-77-0, Iron lanthanum phosphide (Fe4LaP12)  
RL: PRP (Properties)  
(electronic **structure** and thermoelec. prospects of phosphide skutterudites)

REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1998:172328 CAPLUS

DOCUMENT NUMBER: 128:262137

TITLE: Skutterudite vs. ReO3 structures for MX3 solids:  
electronic requirements

AUTHOR(S): Llunell, Miquel; Alvarez, Santiago; Alemany, Pere  
CORPORATE SOURCE: Departament de Quimica Fisica and Departament de Quimica Inorganica, Universitat de Barcelona, Barcelona, 08028, Spain

SOURCE: Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry (1998), (7), 1195-1200  
CODEN: JCDTBI; ISSN: 0300-9246

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Electronic band-structure calcns. on ReO3 and CoP3 were performed to analyze the different structural preferences found for these two compds. The electronic origin of these differences is associated with the formation of the characteristic nonmetal four-membered rings of the skutterudite structure, which is energetically unfavorable for compds. with small, strongly electroneg. anions. The combination of two factors was identified to be responsible for the structural differences between these compds. The 1st is the electronegativity difference between the two types of atoms that form the solid: for strongly electroneg. nonmetal atoms like O or F the ReO3-type structure is expected to be the most stable, while

for the combination of less electroneg. atoms like the pnictides with late transition metals the skutterudite structure is preferred. The 2nd factor is the relative size of the constituting atoms: small atoms like F and O favor the ReO<sub>3</sub> structure, while larger atoms like P and As stabilize the skutterudite one.

IT Crystal structure types

(electronic band structure and electronegativity in relation to stability of skutterudite vs. ReO<sub>3</sub> crystal structure type)

IT Electronegativity

(in relation to stability of skutterudite vs. ReO<sub>3</sub> crystal structure type)

IT Band structure

(of ReO<sub>3</sub> and CoP<sub>3</sub> in relation to stability of skutterudite vs. ReO<sub>3</sub> crystal structure type)

IT 1314-28-9, Rhenium oxide (ReO<sub>3</sub>) 12187-17-6, Cobalt phosphide (CoP<sub>3</sub>)

RL: PRP (Properties)

(electronic band structure and electronegativity in relation to stability of skutterudite vs. ReO<sub>3</sub> crystal structure type)

REFERENCE COUNT: 52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 4 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1996:548108 CAPLUS

DOCUMENT NUMBER: 126:51197

TITLE: Electronic band structure and conductivity of MP<sub>3</sub> (M = Co, Ni) skutterudites

AUTHOR(S): Zhukov, V. P.

CORPORATE SOURCE: Institut Khimii Tverdogo Tela, Yekaterinburg, 620219, Russia

SOURCE: Fizika Tverdogo Tela (Sankt-Peterburg) (1996), 38(1), 166-175

CODEN: FTVTAC; ISSN: 0367-3294

PUBLISHER: Nauka

DOCUMENT TYPE: Journal

LANGUAGE: Russian

AB The electronic band structure was studied of CoP<sub>3</sub> and NiP<sub>3</sub> skutterudites by the Hueckel method. The dependence of the semiconductor gap on the type of A<sub>0</sub> hybridization, electron d. and electron configurations of atoms is determined. The conduction electrons in NiP<sub>3</sub> belong predominantly to the phosphorus sublattice.

IT Band structure

Bond

Density of states

Electric conductivity

Electron configuration

Electron density

(band structure, electron d., and mechanism of conductivity in CoP<sub>3</sub> and NiP<sub>3</sub> skutterudites)

IT 12187-17-6, Cobalt phosphide (CoP<sub>3</sub>) 12192-07-3, Nickel phosphide

(NiP3)

RL: PRP (Properties)

(band structure, electron d., and mechanism of conductivity in CoP3 and NiP3 skutterudites)

L7 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1995:186980 CAPLUS

DOCUMENT NUMBER: 122:13647

TITLE: Promising thermoelectric materials for terrestrial-space applications

AUTHOR(S): Caillat, T.; Borshchevsky, A.; Fleurial, J. P.; Vandersande, J. W.

CORPORATE SOURCE: Jet Propulsion Laboratory, California Institute Technology, Pasadena, CA, 91109, USA

SOURCE: Proceedings of the Intersociety Energy Conversion Engineering Conference (1994), 29TH(PT. 1), 575-9  
CODEN: PIECDE; ISSN: 0146-955X

DOCUMENT TYPE: Journal

LANGUAGE: English

AB This paper presents a new family of materials with the skutterudite crystal structure which, based on initial results obtained on several compds. of this family, has a good potential for thermoelec. applications. This class of materials covers a wide range of decomposition temps. and bandgaps, which could be used for low, intermediate to high temperature applications. The interesting features of the skutterudite family of materials are discussed.

IT Thermoelectric materials

(thermoelec. materials with skutterudite crystal structure for terrestrial-space applications)

IT 12187-17-6, Cobalt phosphide (CoP3) 12187-20-1, Cobalt antimonide (CoSb3) 12192-07-3, Nickel phosphide (NiP3) 12196-58-6, Iridium phosphide (IrP3) 12196-60-0, Iridium antimonide (IrSb3) 12202-47-0, Palladium phosphide (PdP3) 12202-48-1, Rhodium phosphide (RhP3) 12210-72-9, Rhodium antimonide (RhSb3) 12256-04-1, Cobalt arsenide (CoAs3) 12256-08-5, Iridium arsenide (IrAs3) 12256-11-0, Rhodium arsenide (RhAs3)

RL: PRP (Properties); TEM (Technical or engineered material use); USES (Uses)

(with skutterudite crystal structure; as thermoelec. material for terrestrial-space applications)

L7 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1978:30582 CAPLUS

DOCUMENT NUMBER: 88:30582

TITLE: The preparation and characterization of the cobalt skutterudites 1:3 cobalt pnictide compounds

AUTHOR(S): Ackermann, J.; Wold, A.

CORPORATE SOURCE: Dep. Chem., Brown Univ., Providence, RI, USA

SOURCE: Journal of Physics and Chemistry of Solids (1977), 38(9), 1013-16

CODEN: JPCSAW; ISSN: 0022-3697

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The crystal structures of  $\text{CoX}_3$  ( $X = \text{P, As, Sb}$ ), prepared by chemical vapor transport with  $\text{Cl}_2$  as the transport agent, were determined by x-ray diffraction; the space group is  $\text{IM}\bar{3}$  and  $a_0 = 7.702, 8.208, \text{ and } 9.034 \text{ \AA}$ , resp. The crystal stoichiometries are  $\text{Co}_{1.001}\text{X}_{3.001}$ . The magnetic susceptibilities indicate diamagnetic behavior. Hall and Seebeck effects and elec. resistances were also determined.  $\text{CoP}_3$  is a semiconductor with an optical band gap of 0.45 eV.  $\text{CoSb}_3$  and  $\text{CoAs}_3$  have no band gaps and their resistivities increase with temperature. A band diagram for  $\text{CoAs}_3$  is proposed, based on a 1-electron scheme for other transition metal chalcogenides and pnictides.

IT Semiconductor materials  
(cobalt tripnictides)

IT Crystal structure  
Electric resistance  
Hall effect  
Magnetic susceptibility  
Thermoelectricity  
(of cobalt pnictides)

IT Energy level, band structure  
(of cobalt tripnictides)

IT Magnetic property and Magnetism  
(dia-, of cobalt pnictides)

IT Energy level, band structure  
(gap, of cobalt phosphide)

IT Crystal structure types  
(skutterudite, of cobalt pnictides, elec. and magnetic properties of)

IT 12187-17-6 12187-20-1 12256-04-1

RL: PRP (Properties)

(crystal structure and elec. and magnetic properties of)

L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1969:32440 CAPLUS

DOCUMENT NUMBER: 70:32440

TITLE: Structure and bonding in skutterudite-type phosphides

AUTHOR(S): Rundqvist, Stig; Ersson, Nils O.

CORPORATE SOURCE: Univ. Uppsala, Uppsala, Swed.

SOURCE: Arkiv foer Kemi (1968), 30(10), 103-14

CODEN: ARKEAD; ISSN: 0365-6128

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The crystal structures of  $\text{CoP}_3$ ,  $\text{RhP}_3$ ,  $\text{IrP}_3$ , and  $\text{NiP}_3$  were determined by x-ray powder diffraction methods. The metal atoms have a distorted octahedral environment of 6 P atoms, the Co-P, Rh-P, Ir-P, and Ni-P distances being 2.22, 2.34, 2.34, and 2.38 Å, resp. The P atoms form planar, rectangular  $\text{P}_4$  groups with P-P distances along the shorter edges of 2.22-2.24 Å and along the longer edges of 2.28-2.34 Å. Different schemes for the chemical bonding are reviewed and discussed in relation to the elec. and magnetic



- properties of the compds.
- IT Crystal structure  
(of phosphides)
- IT Iridium phosphide (IrP3)  
Phosphide  
Rhodium phosphide (RhP3)  
RL: PRP (Properties)  
(crystal structure of)
- IT 12187-17-6 12192-07-3  
RL: PRP (Properties)  
(crystal structure of)

L7 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1966:31876 CAPLUS

DOCUMENT NUMBER: 64:31876

ORIGINAL REFERENCE NO.: 64:5894b-d

TITLE: Electron-valence diagram for semiconductor compounds  
of the skutterudite type

AUTHOR(S): Kuz'min, R. N.

SOURCE: Khim. Svyaz v Poluprov. i Tverd. Telakh, Inst. Fiz.  
Tverd. Tela i Poluprov., Akad. Nauk Belorussk. SSR  
(1965) 335-46

DOCUMENT TYPE: Journal

LANGUAGE: Russian

AB cf. CA 64, 4403g. The structure of compds. AVIIB3V with structures of  
the skutterudite type was analyzed. Of the BV elements, As and Sb for AB3  
compds. only with Co, Rh, and Ir, whereas P forms compds. of this type  
also with Ni and Pd. N and Bi do not form compds. of the skutterudite  
type. A model taking into account the presence of the sq. radical [B]4  
was suggested. Only in this respect did the suggested model differ from  
the scheme suggested by Dudkin (D. and Abrikosov, CA 53, 14706c; D., CA  
53, 19582e). In the compound CoSb3, all valence shells of Sb and Co  
participate in the formation of hybrid functions d2sp3 and sp3. This  
modified scheme agreed with exptl. data.

- IT Electrons  
(configuration or d. distribution of, of antimonides, arsenides and  
phosphides of Group VIII metals with skutterudite structure)
- IT Crystal structure  
(of antimonides, arsenides and phosphides of Group VIII metals with  
skutterudite structure)
- IT 12187-17-6, Cobalt phosphide, CoP3 12187-20-1, Cobalt  
antimonide, CoSb3 12192-07-3, Nickel phosphide, NiP3 12196-58-6,  
Iridium phosphide, IrP3 12196-60-0, Iridium antimonide, IrSb3  
12202-47-0, Palladium phosphide, PdP3 12202-48-1, Rhodium phosphide,  
RhP3 12210-72-9, Rhodium antimonide, RhSb3 12256-04-1, Cobalt  
arsenide, CoAs3 12256-08-5, Iridium arsenide, IrAs3  
(crystal structure and electron configuration of)

L7 ANSWER 9 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1963:401987 CAPLUS

DOCUMENT NUMBER: 59:1987  
ORIGINAL REFERENCE NO.: 59:278c-f  
TITLE: Crystallochemical characteristics of borides,  
nitrides, silicides, and phosphides of transition  
metals  
AUTHOR(S): Samsonov, G. V.  
SOURCE: Poroshkovaya Met., Akad. Nauk Ukr. SSR (1963), 3(No.  
2), 65-79  
DOCUMENT TYPE: Journal  
LANGUAGE: Unavailable

AB The principal factors which determine the character of the crystal lattice and phys. properties of the compds. studied are: (1) relative dimensions of the metal and nonmetal atoms, (2) degree of electronegativity, (3) ionization potential of the nonmetallic atom, (4) electron affinity and degree of filling of incomplete shells of the metal atoms. These factors were compared and correlated and the following classification of the compds. studied was made. Nitrides of Ti, Zr, Hf, and V with stoichiometric composition show metallic properties, while nitrides of Mo and W represent ionic compds. On the other hand, nitrides of Nb, Ta, and Cr combine metallic and ionic bonds, with some predominance of the latter. Borides are characterized by the presence of isolated configurations of B atoms which become more complicated as B content in borides increases. Hexaborides can be divided into 2 groups (according to their thermal conductivity): (a) Y, La, Ca, Sr, and Ba, in which conductivity increases (in the given

order) slowly with increase in atomic radius; (b) Sm, Nd, Ce, Pr, Ta, Th, and Gd, in which thermal conductivity increases sharply (in the given order) with lowered atomic radius. Yb and Eu are the exceptions in this classification. The majority of silicides represent metallic properties except for Mn, Cr, Fe, and Re, which show semiconductor properties. Phosphides show the highest degree of metallicity of bonds and their heats of formation are lower than those of nitrides. However, because of the ability of P atoms to form covalent bonds with each other, the heats of formation of carbides are lower than those of phosphides, while with increased number of P atoms per atom of metal the heat of formation increases.

IT Electrons

(configuration or d. distribution of, in transition metal borides, nitrides, phosphides and silicides)

IT Transition metal borides

Transition metal carbides

Transition metal nitrides

Transition metal phosphides

Transition metal silicides

(crystal structure and phys. properties of)

IT Bonds

(in transition metal borides, nitrides, phosphides and silicides)

IT Crystal structure

(of transition metal borides, nitrides, phosphides and silicides)

IT Heat of formation

(of transition metal borides, nitrides, phosphides and silicides,

- crystal structure and)
- IT Conductivity, thermal and(or) Conduction, thermal  
(of transition metal hexaborides, crystal structure and)
- IT Electronegativity  
(of transition metals, in crystal structure and phys. properties of  
transition metal borides, nitrides, phosphides and silicides)
- IT Semiconductors, electric  
(transition metal silicides as)
- IT Calcium boride silicide  
Calcium silicide boride  
Niobium nitride  
Tantalum nitride  
Titanium silicide, TiSi  
Vanadium nitride  
(crystal structure and phys. properties of)
- IT 1310-43-6, Iron phosphide, FeP 11103-55-2, Nickel phosphide, Ni<sub>5</sub>P<sub>2</sub>  
12007-99-7, Calcium boride, CaB<sub>6</sub> 12008-02-5, Cerium boride, CeB<sub>6</sub>  
12008-05-8, Europium boride, EuB<sub>6</sub> 12008-06-9, Gadolinium boride, GdB<sub>6</sub>  
12008-21-8, Lanthanum boride, LaB<sub>6</sub> 12008-23-0, Neodymium boride, NdB<sub>6</sub>  
12008-27-4, Praseodymium boride, PrB<sub>6</sub> 12008-30-9, Samarium boride, SmB<sub>6</sub>  
12008-31-0, Terbium boride, TbB<sub>6</sub> 12008-32-1, Yttrium boride, YB<sub>6</sub>  
12008-33-2, Ytterbium boride, YbB<sub>6</sub> 12017-11-7, Cobalt silicide, CoSi  
12017-12-8, Cobalt silicide, CoSi<sub>2</sub> 12018-08-5, Chromium silicide, CrSi  
12018-09-6, Chromium silicide, CrSi<sub>2</sub> 12018-36-9, Chromium silicide,  
Cr<sub>3</sub>Si 12022-85-4, Iron phosphide, FeP<sub>2</sub> 12022-95-6, Iron silicide, FeSi  
12022-99-0, Iron silicide, FeSi<sub>2</sub> 12023-53-9, Iron phosphide, Fe<sub>3</sub>P  
12023-54-0, Iron silicide, Fe<sub>3</sub>Si 12032-85-8, Manganese silicide, MnSi  
12032-86-9, Manganese silicide, MnSi<sub>2</sub> 12033-37-3, Molybdenum silicide,  
Mo<sub>3</sub>Si 12033-40-8, Molybdenum silicide, Mo<sub>5</sub>Si<sub>3</sub> 12033-43-1, Niobium  
nitride, Nb<sub>2</sub>N 12033-62-4, Tantalum nitride, TaN 12033-63-5, Tantalum  
nitride, Ta<sub>2</sub>N 12035-47-1, Nickel phosphide, NiP<sub>2</sub> 12035-64-2, Nickel  
phosphide, Ni<sub>2</sub>P 12037-65-9, Titanium phosphide, TiP 12038-66-3,  
Rhenium silicide, ReSi<sub>2</sub> 12039-75-7, Vanadium silicide, VSi 12039-79-1,  
Tantalum silicide, TaSi<sub>2</sub> 12039-88-2, Tungsten silicide, WSi<sub>2</sub>  
12039-90-6, Zirconium silicide, ZrSi<sub>2</sub> 12046-08-1, Barium boride, BaB<sub>6</sub>  
12046-54-7, Strontium boride, SrB<sub>6</sub> 12052-37-8, Cobalt phosphide, CoP  
12053-27-9, Chromium nitride, Cr<sub>2</sub>N 12059-22-2, Nickel silicide, Ni<sub>3</sub>Si  
12067-56-0, Tantalum silicide, Ta<sub>5</sub>Si<sub>3</sub> 12134-02-0, Cobalt phosphide, Co<sub>2</sub>P  
12134-19-9, Chromium silicide, Cr<sub>3</sub>Si<sub>2</sub> 12136-78-6, Molybdenum silicide,  
MoSi<sub>2</sub> 12163-59-6, Manganese silicide, Mn<sub>3</sub>Si 12187-17-6, Cobalt  
phosphide, CoP<sub>3</sub> 12192-07-3, Nickel phosphide, NiP<sub>3</sub> 12201-89-7, Nickel  
silicide, NiSi<sub>2</sub> 12229-63-9, Thorium boride, ThB<sub>6</sub> 12396-85-9, Nickel  
silicide, Ni<sub>3</sub>Si<sub>2</sub> 12410-47-8, Cobalt silicide, Co<sub>3</sub>Si 12413-09-1,  
Tantalum silicide, Ta<sub>4</sub>Si 12504-62-0, Tungsten silicide, W<sub>3</sub>Si  
12705-37-2, Chromium nitride 24094-93-7, Chromium nitride, CrN  
24621-21-4, Niobium nitride, NbN 24646-85-3, Vanadium nitride, VN  
25583-20-4, Titanium nitride, TiN 25658-42-8, Zirconium nitride, ZrN  
26508-33-8, Iron phosphide, FeP 37245-81-1, Molybdenum nitride  
(crystal structure and phys. properties of)

